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Notice of Allowance: March 8, 2004
Application No.: 09/629,557

Our Ref. No. 4239-55412
First Named Inventor: Miller et al.
For: METHODS FOR PREDICTING THE BIOLOGICAL,
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Confirmation No. 4093
Filed: July 31, 2000

Replacement Sheet (Sheet 1 of 31)

SDBS- ^{13}C NMR SDBS No. 1716CDS-12-007

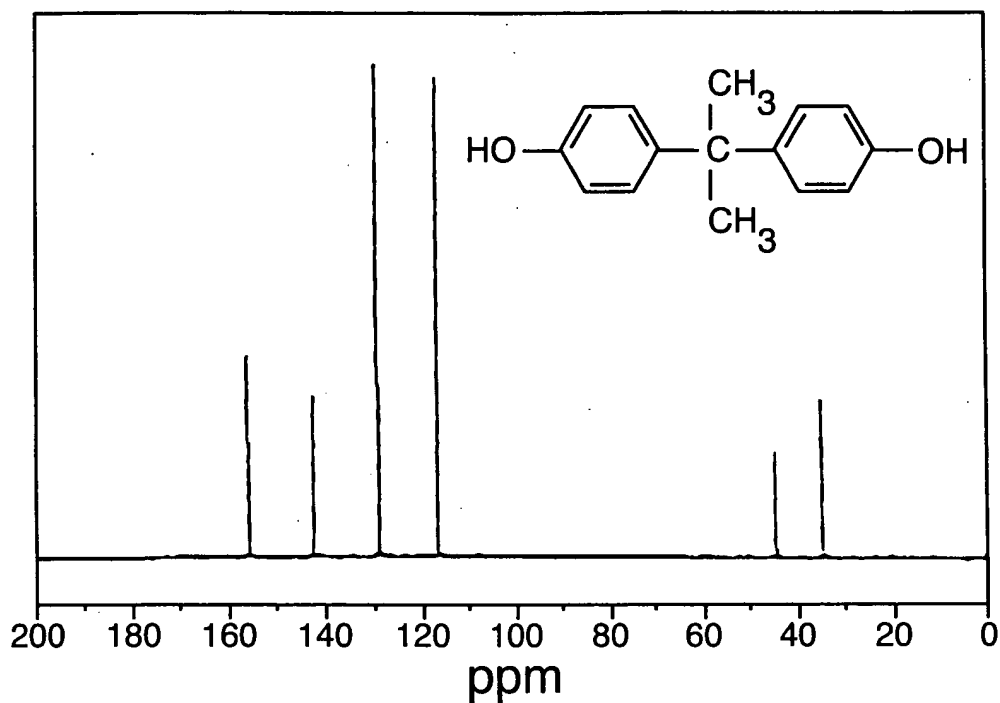
$\text{C}_{15}\text{H}_{16}\text{O}_2$

4, 4' - ISOPROPYLIDENEDIPHENOL

FIG. 1(a)

22.53 MHz

0.025 g : 0.5 ml DMSO- d_5



SDBS-Mass

MS-NW-6834 SDBS No. - 1716
4, 4' - ISOPROPYLIDENEDIPHENOL
(Mass of molecular ion: 228)

FIG. 1(b)

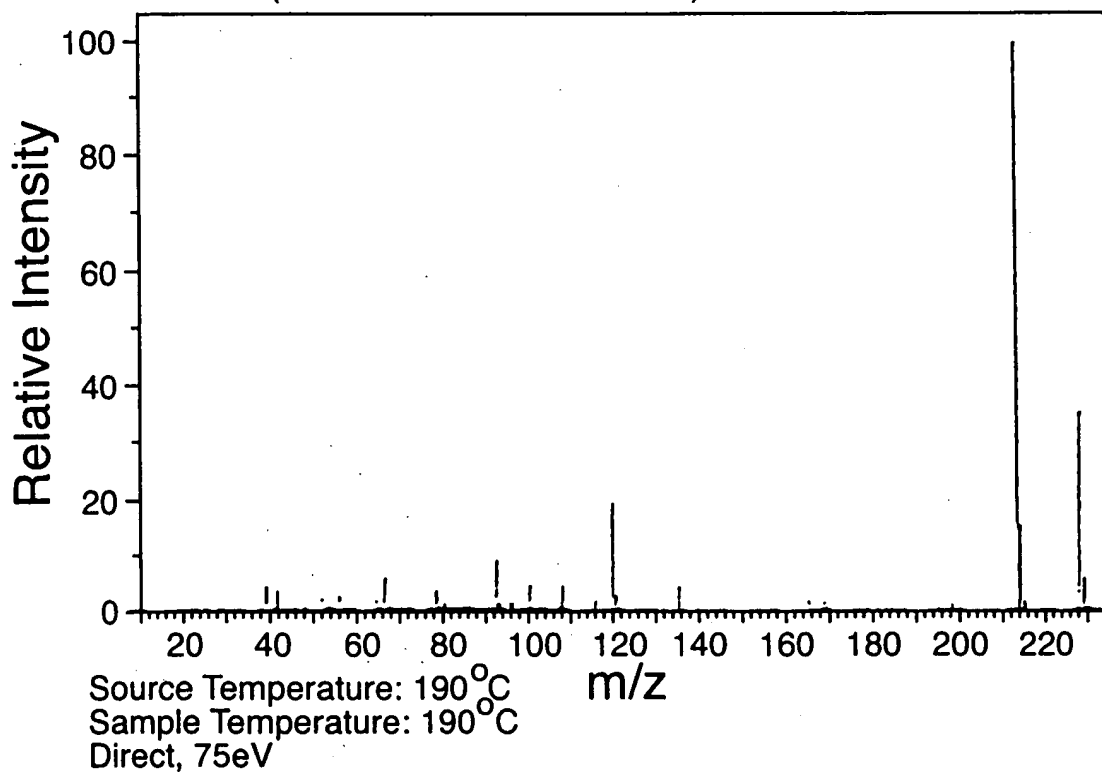
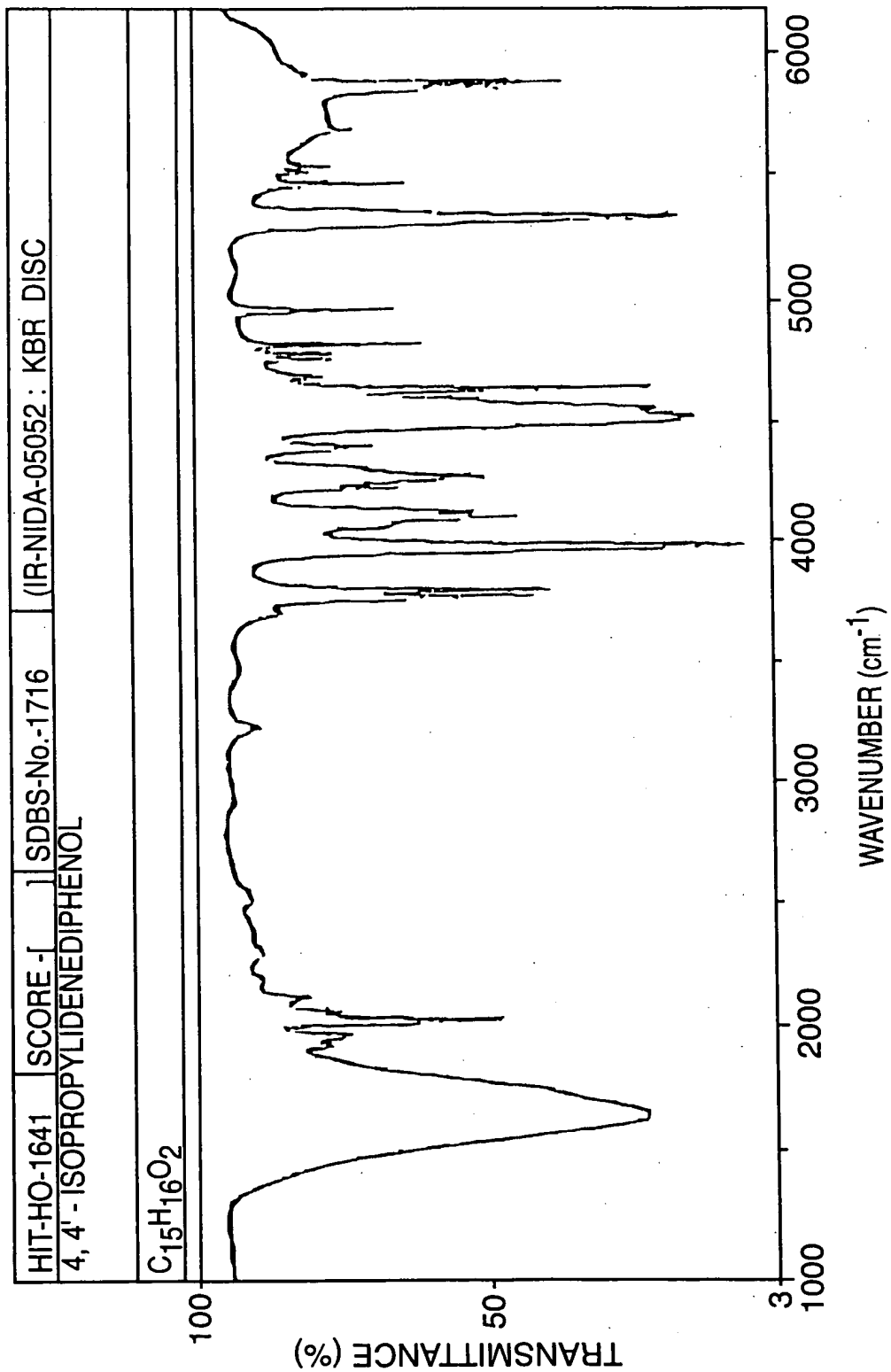


FIG. 1(c)



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Replacement Sheet (Sheet 2 of 31)

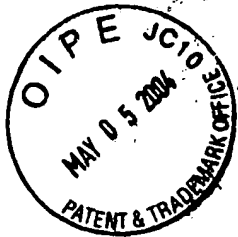
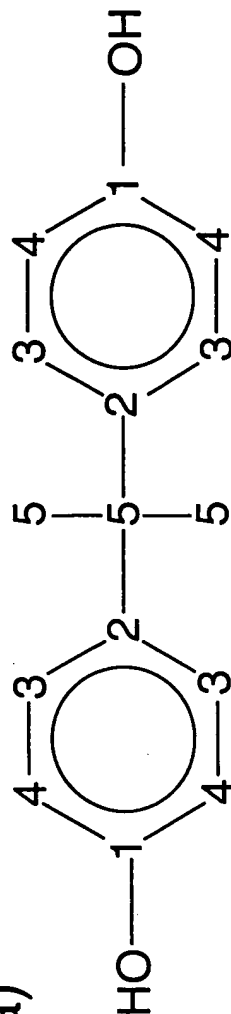
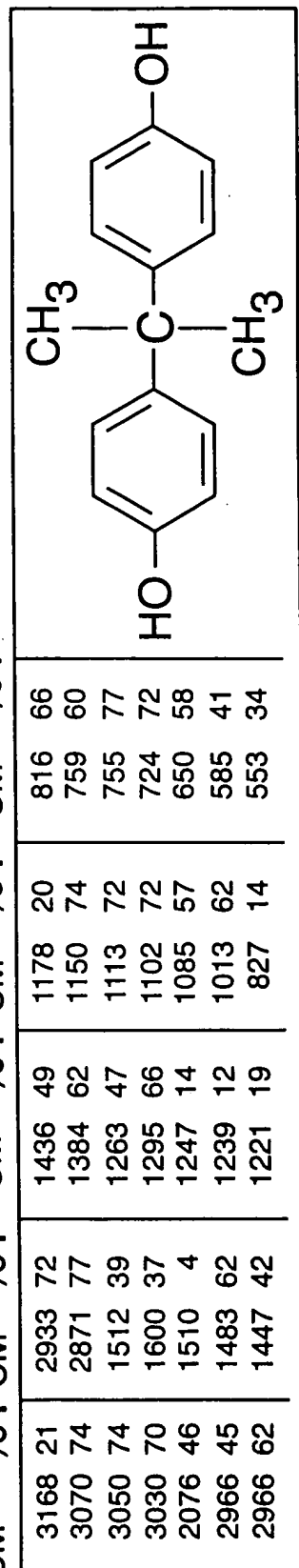


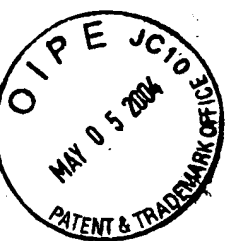
FIG. 2(a)



^{13}C	δ	ppm	Int.	Assign.
		154.72	411	1
		140.94	330	2
		127.11	1000	3
		114.43	977	4
		40.78	223	5
		30.73	328	6

FIG. 2(c)

 $\text{cm}^{-1} \quad \%T \quad \text{cm}^{-1} \quad \%T \quad \text{cm}^{-1} \quad \%T \quad \text{cm}^{-1} \quad \%T$ 



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Replacement Sheet (Sheet 4 of 31)

SDBS-Mass

FIG. 2(b)

MS-NW-6834

SDBS NO. - 1716

4, 4' - ISOPROPYLIDENEDIPHENOL

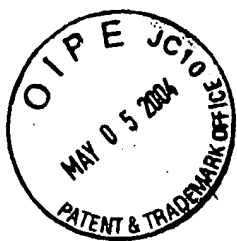
$C_{15}H_{16}O_2$

/Mass of molecular ion:

228:

m/z ratio

27.0	1
39.0	4
41.0	3
51.0	2
55.0	2
63.0	2
65.0	5
66.0	1
76.0	1
77.0	3
79.0	1
89.0	1
90.0	1
91.0	9
92.0	1
94.0	2
95.0	1
99.0	4
105.0	1
106.5	2
107.0	4
114.0	1
115.0	1
119.0	19
120.0	2
134.0	1
135.0	4
152.0	1
165.0	2
169.0	1
181.0	1
183.0	1
195.0	1
197.0	1
198.0	1
212.0	1
213.0	100
214.0	15
215.0	1
229.0	35
239.0	5



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Replacement Sheet (Sheet 5 of 31)

Bin Number	Spectral Intensity	Bin Number	Spectral Intensity	Bin Number	Spectral Intensity
51	2	183	1	1025	62
55	2	195	1	1026	42
63	2	197	1	1027	49
65	5	198	1	1032	62
66	1	212	1	1034	47
76	1	213	100	1041	66
77	3	214	15	1046	14
79	1	215	1	1047	12
89	1	228	35	1048	19
90	1	229	5	1053	20
91	9	580	328	1056	74
92	1	590	223	1059	72
94	2	664	977	1060	72
95	1	677	1000	1062	57
99	4	690	330	1069	62
105	1	704	441	1088	14
106	2	834	21	1089	55
107	4	864	74	1095	60
114	1	866	74	1097	77
115	1	868	70	1098	72
119	19	873	46	1106	68
120	2	874	46	1114	41
134	1	875	62	1115	34
135	4	877	72		
152	1	883	77		
165	2	1009	39		
169	1	1011	37		
181	1	1019	4		

FIG. 3 – a hypothetical set of spectrally derived molecular structure descriptors for bisphenol A.

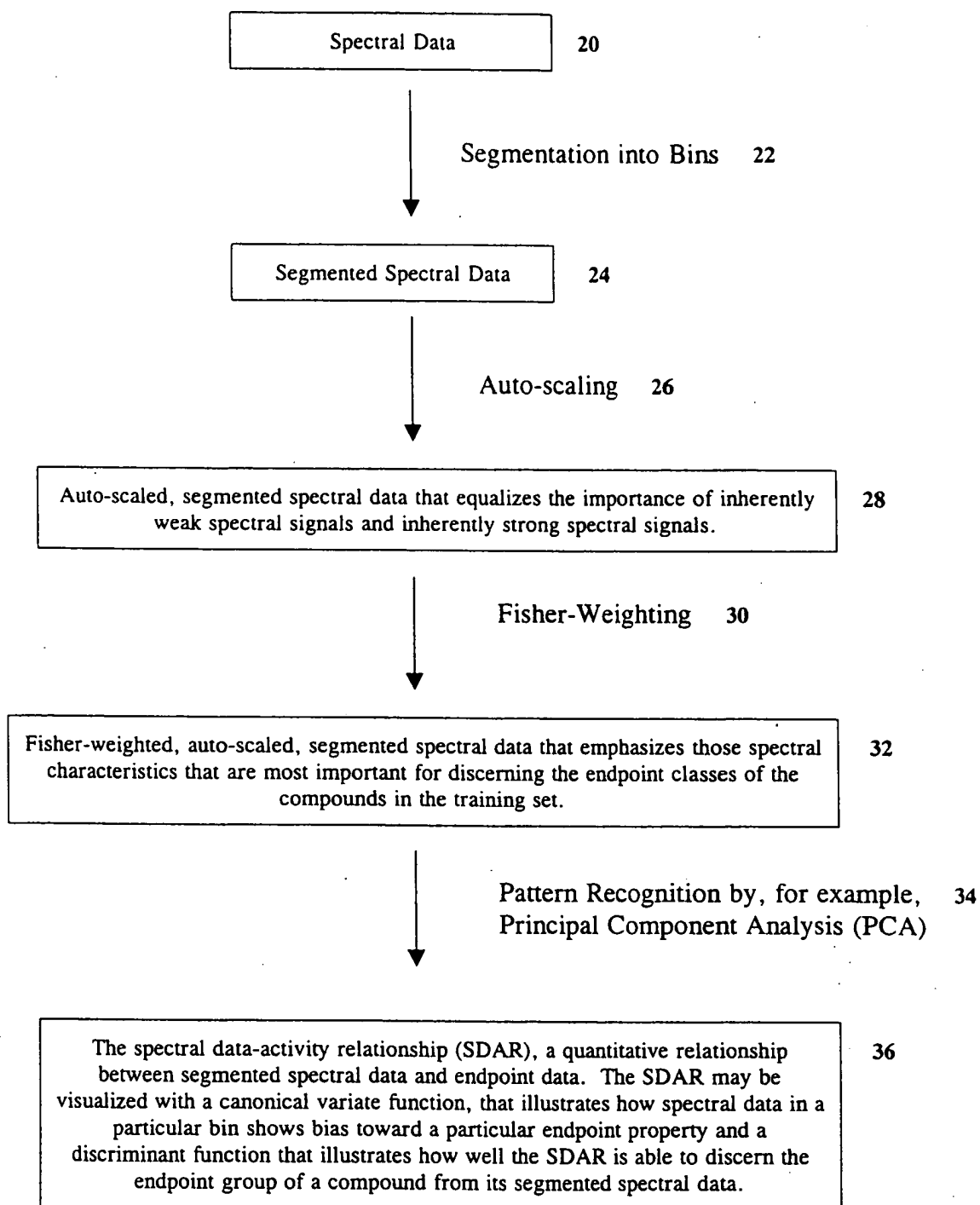
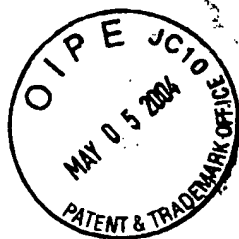
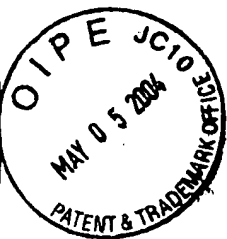


FIG. 4



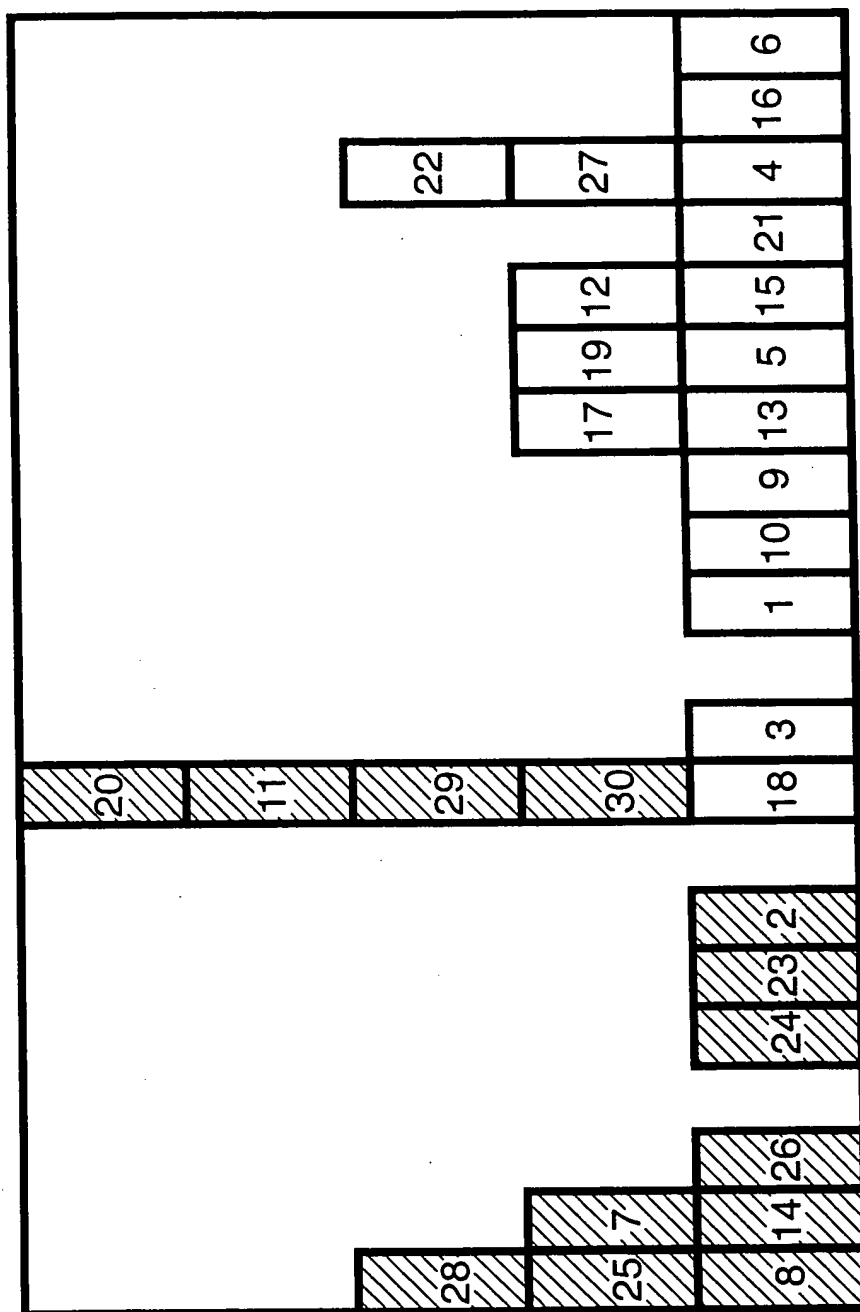
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Replacement Sheet (Sheet 7 of 31)

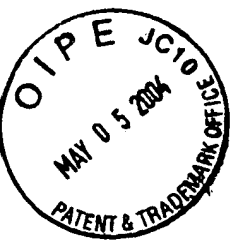
DISCRIMINANT FUNCTION

FIG. 5



Component 1

Component Frequency



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Replacement Sheet (Sheet 8 of 31)

CANONICAL VARIATE 1

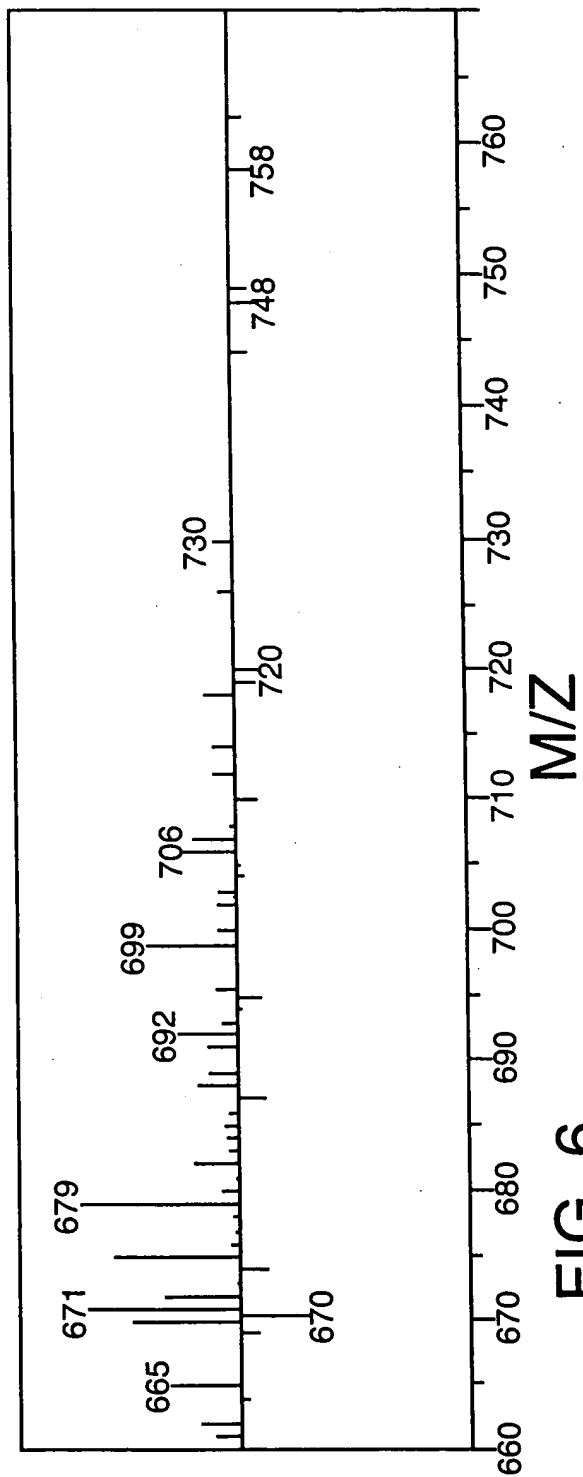
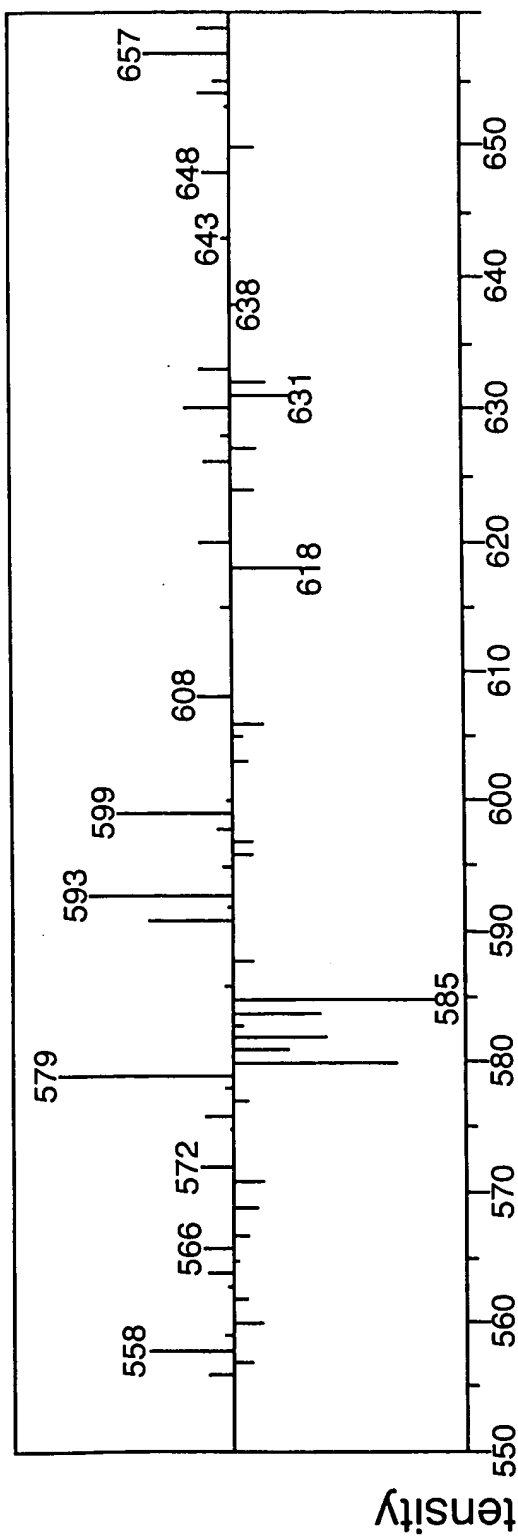
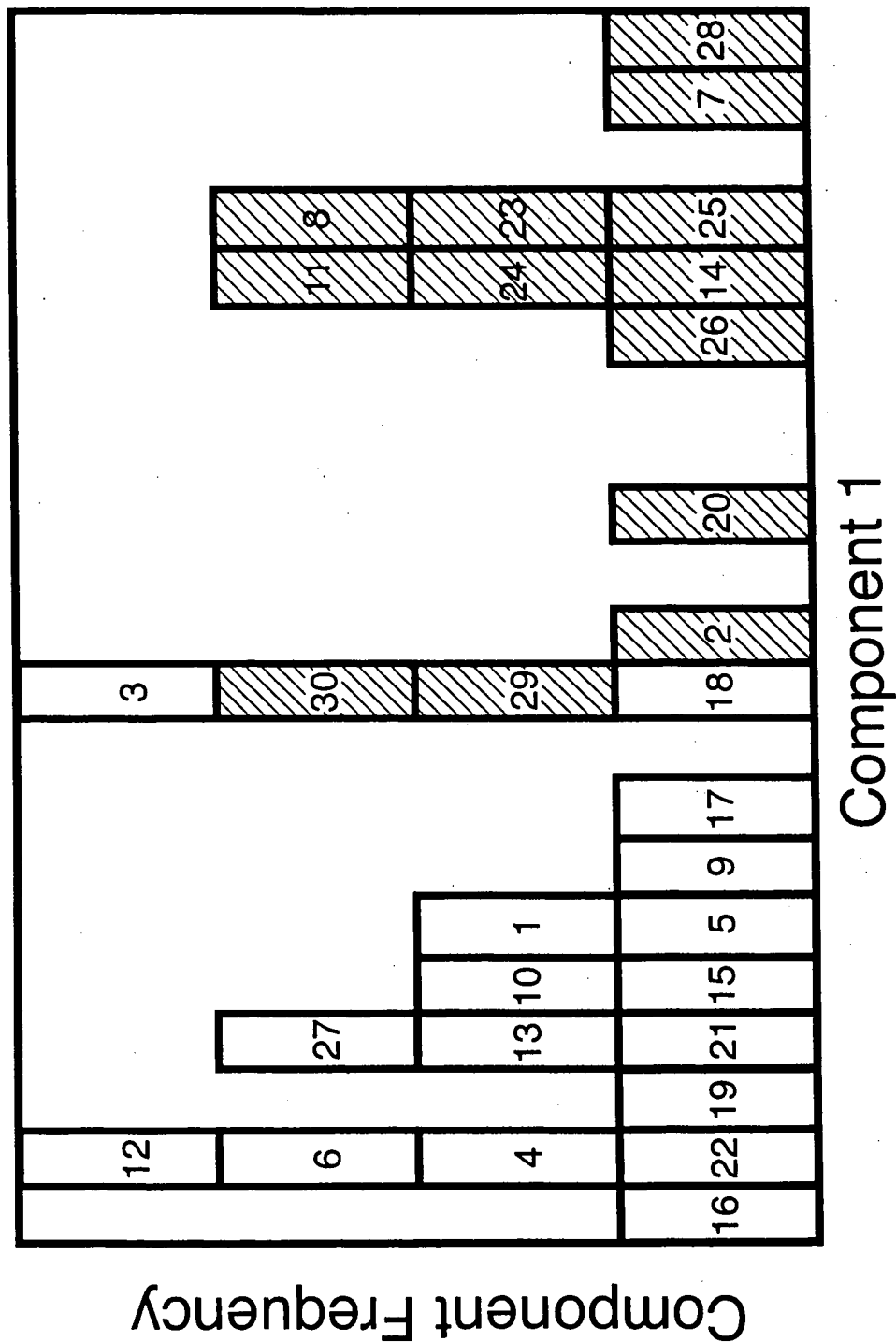


FIG. 6

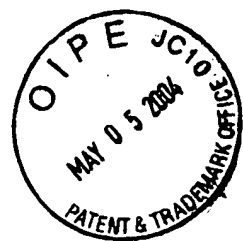
FIG. 7 DISCRIMINANT FUNCTION

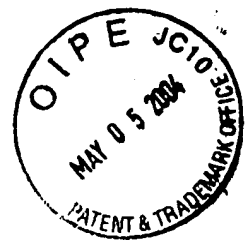


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Replacement Sheet (Sheet 9 of 31)





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Replacement Sheet (Sheet 10 of 31)

CANONICAL VARIATE 1

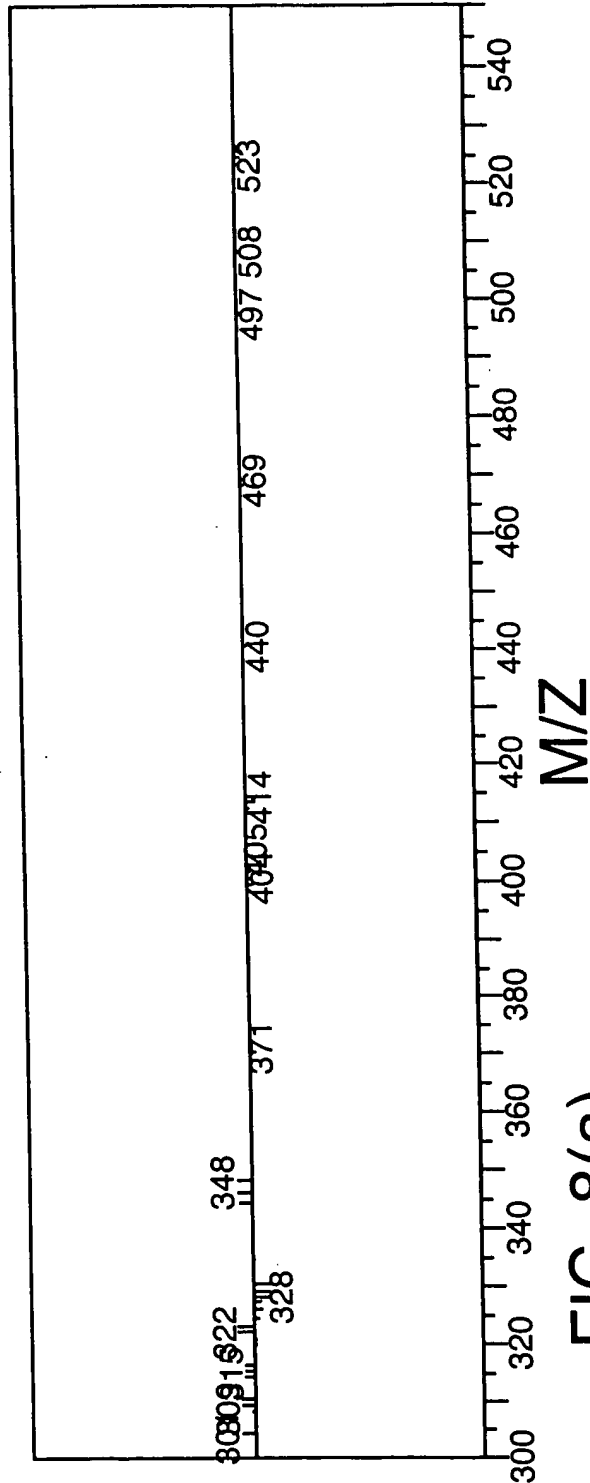
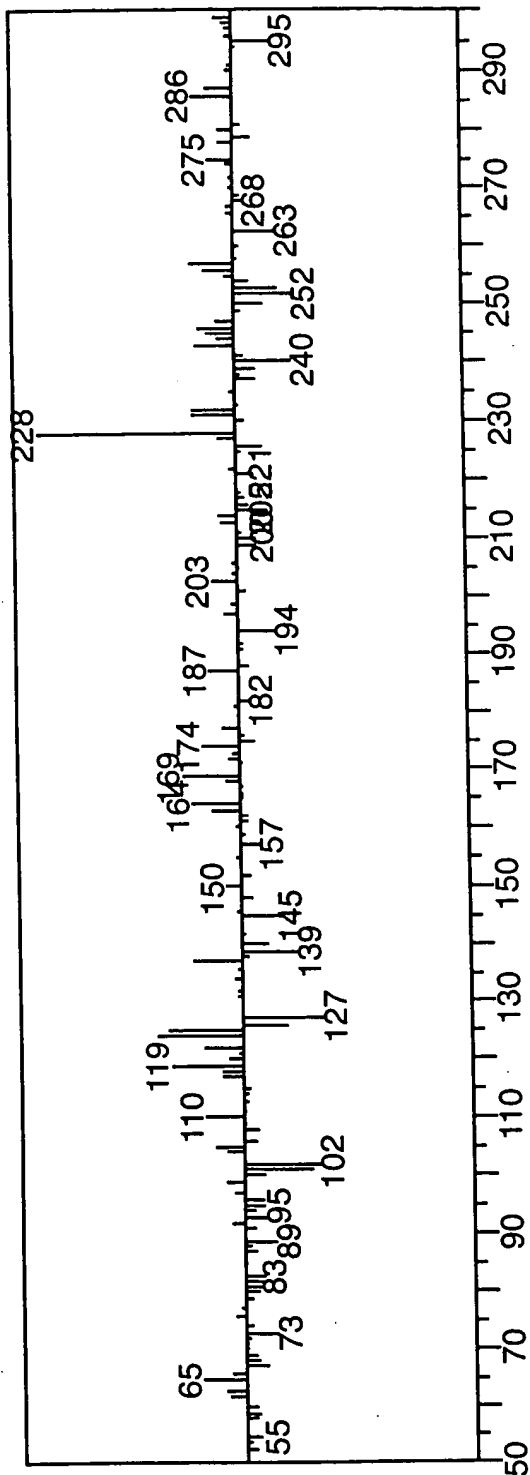
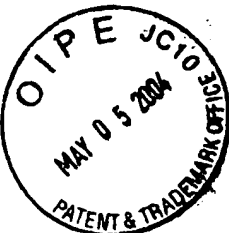


FIG. 8(a)

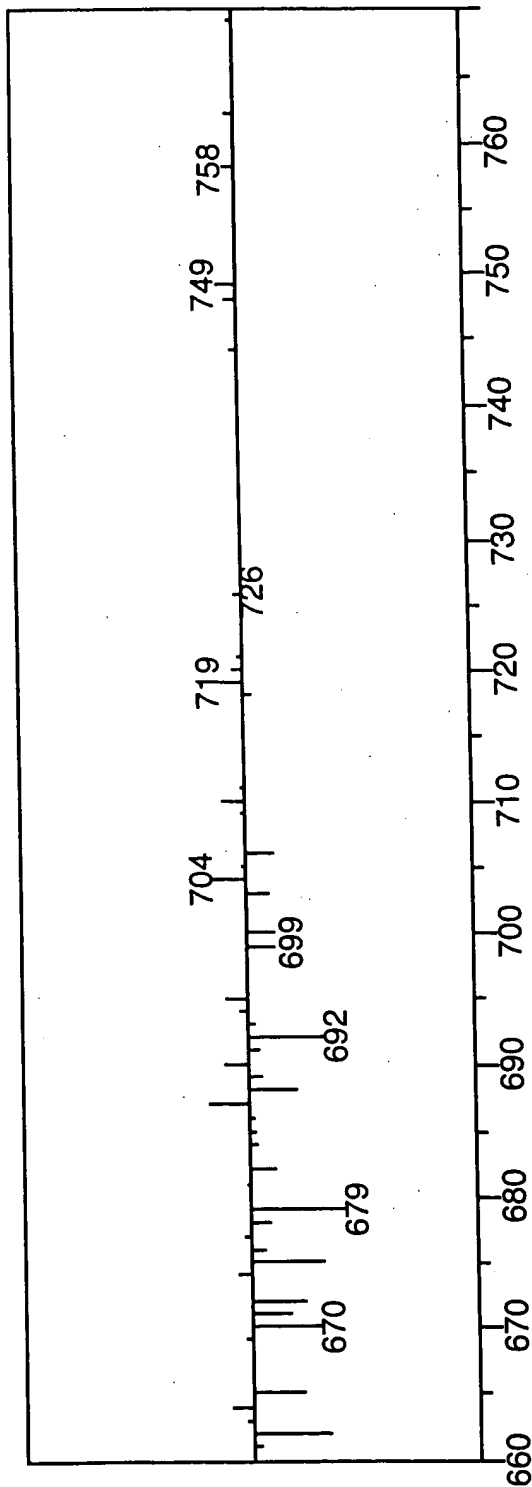
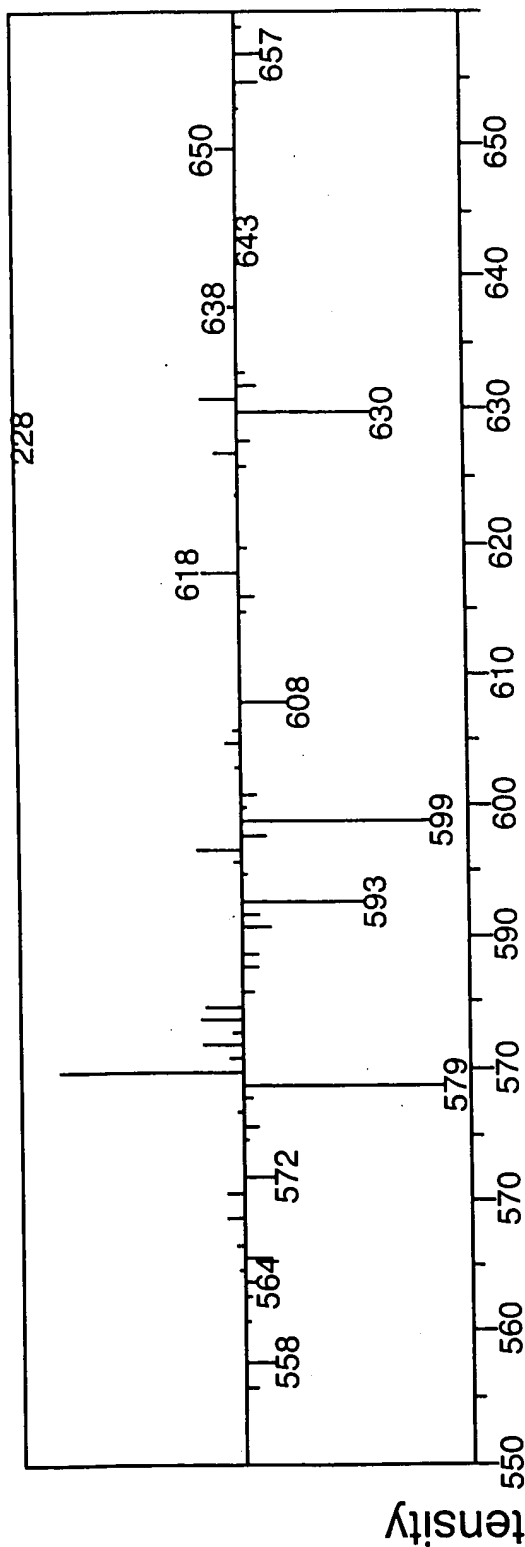


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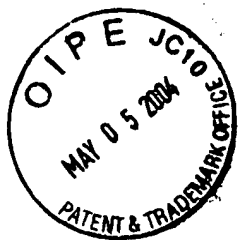
Replacement Sheet (Sheet 11 of 31)

CANONICAL VARIATE 1



M/Z

FIG. 8(b)

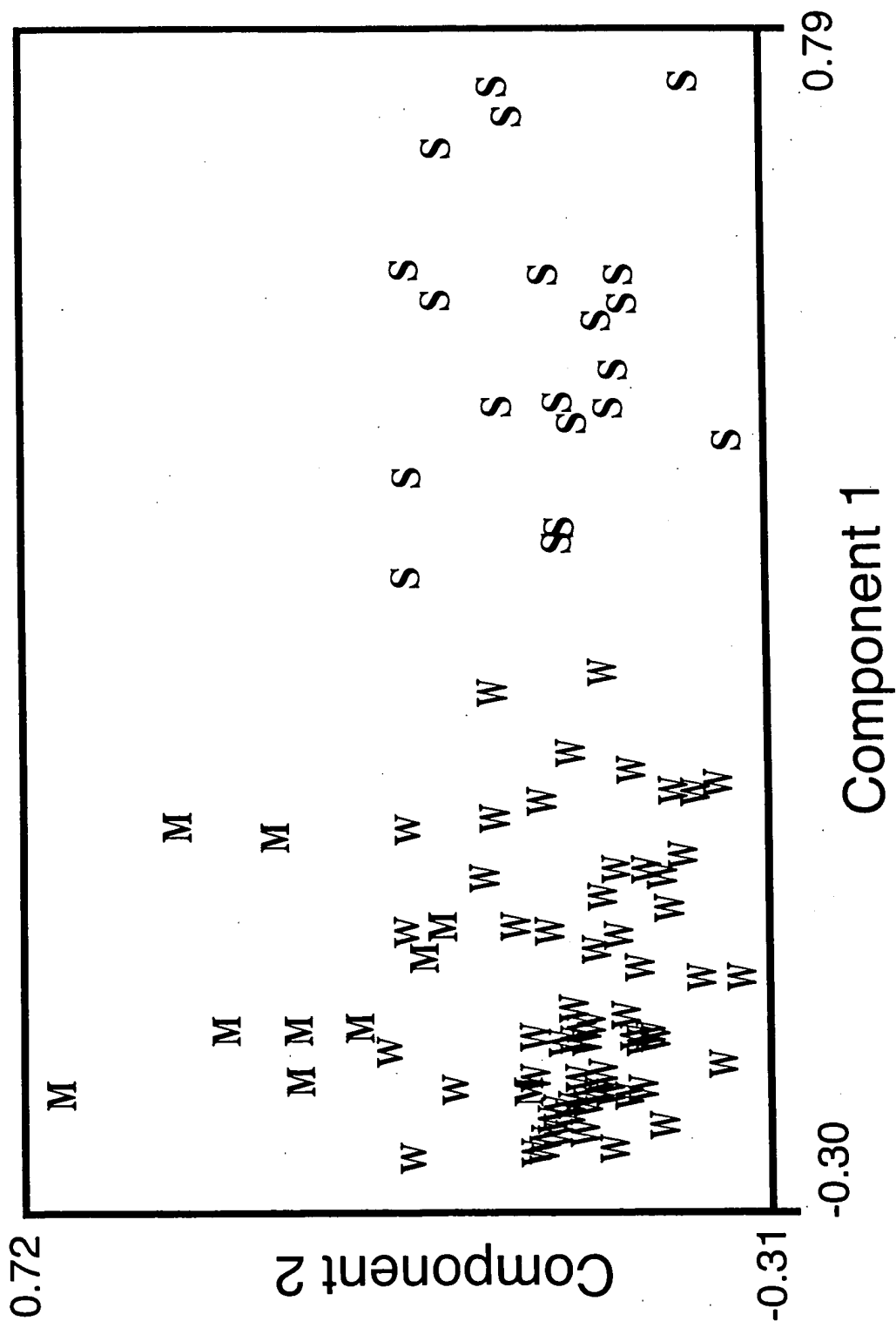


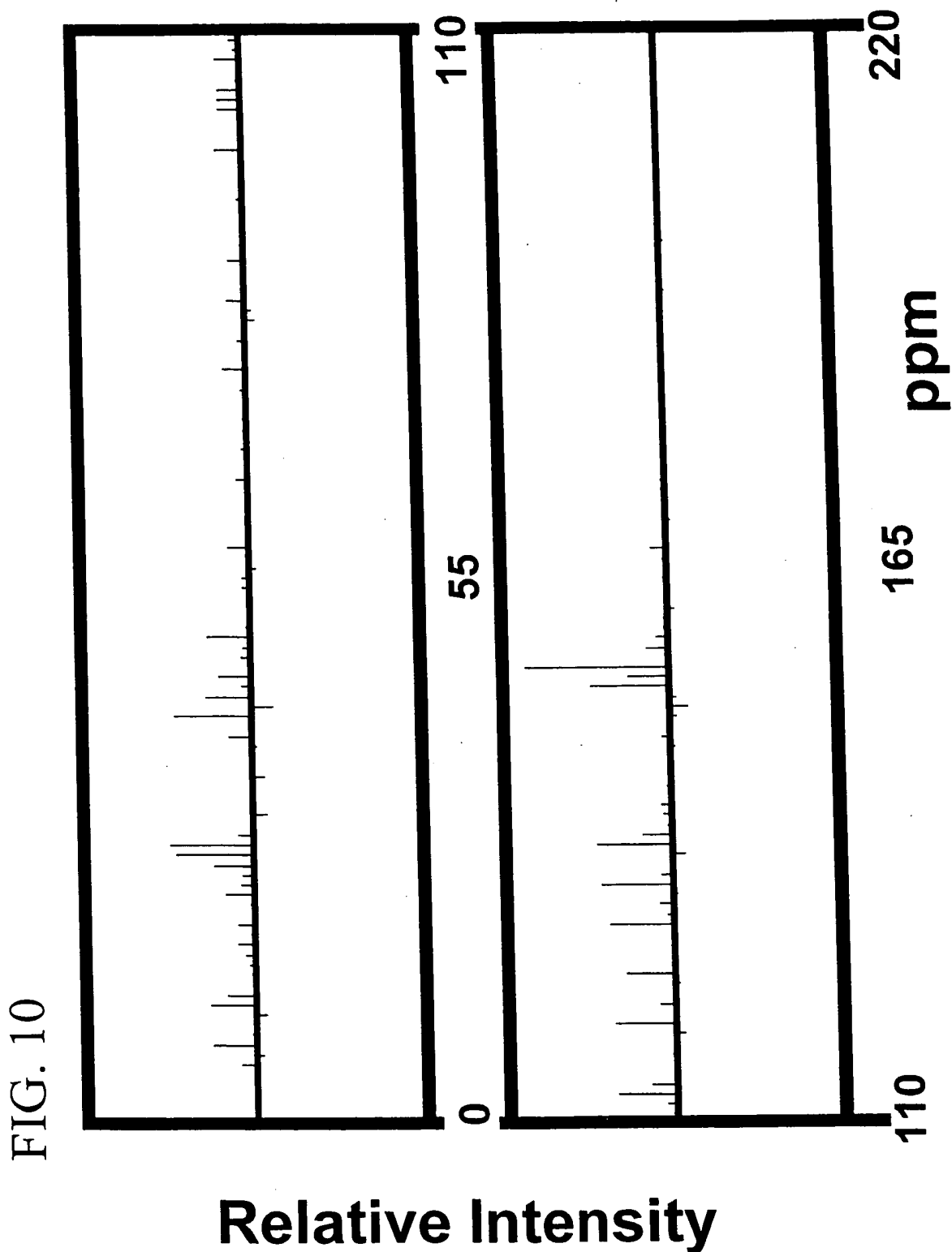
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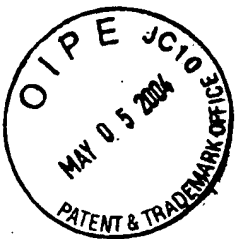
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Replacement Sheet (Sheet 12 of 31)

FIG. 9





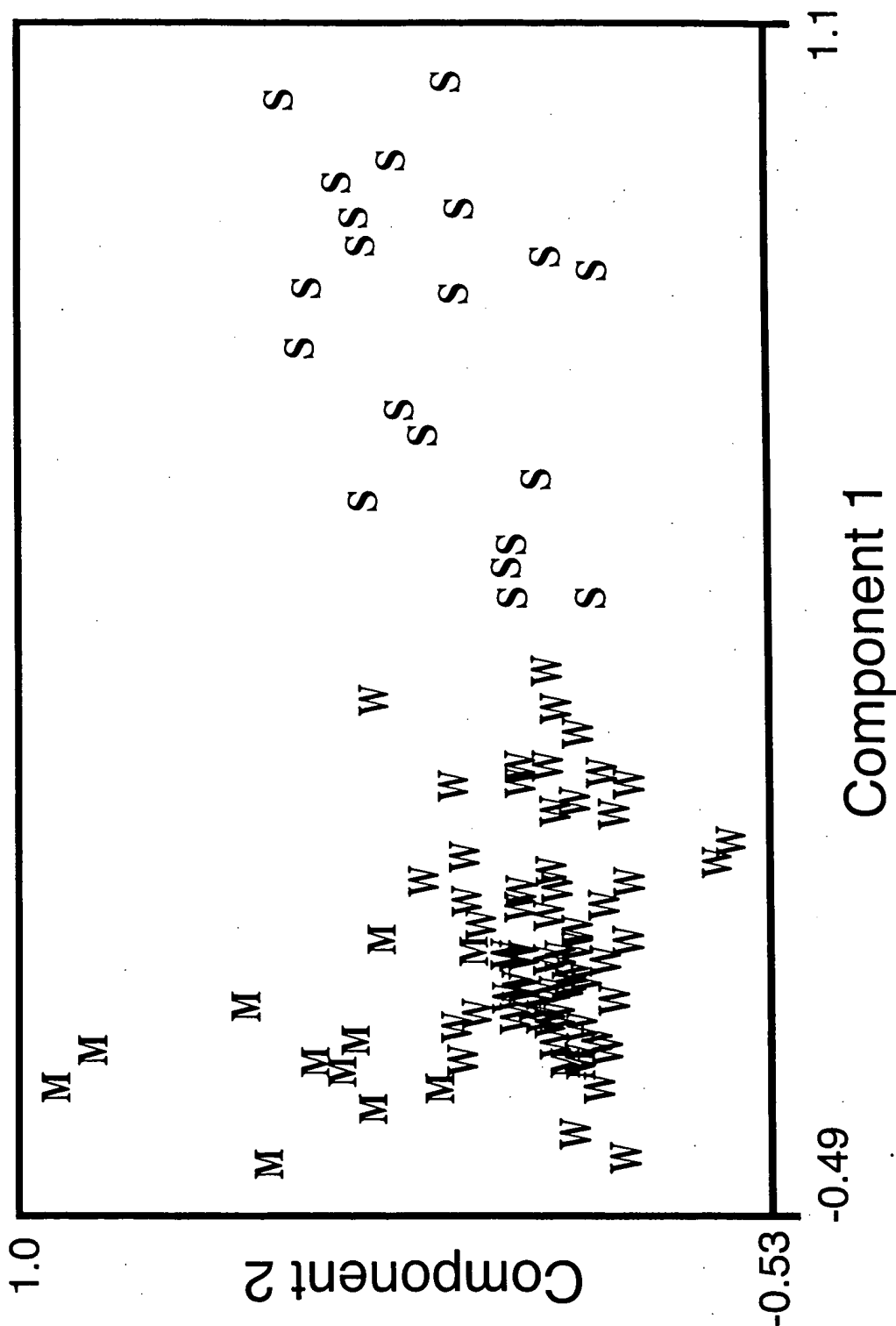


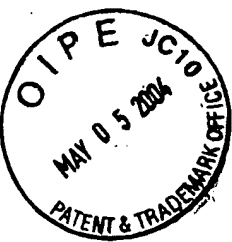
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Replacement Sheet (Sheet 14 of 31)

FIG. 11



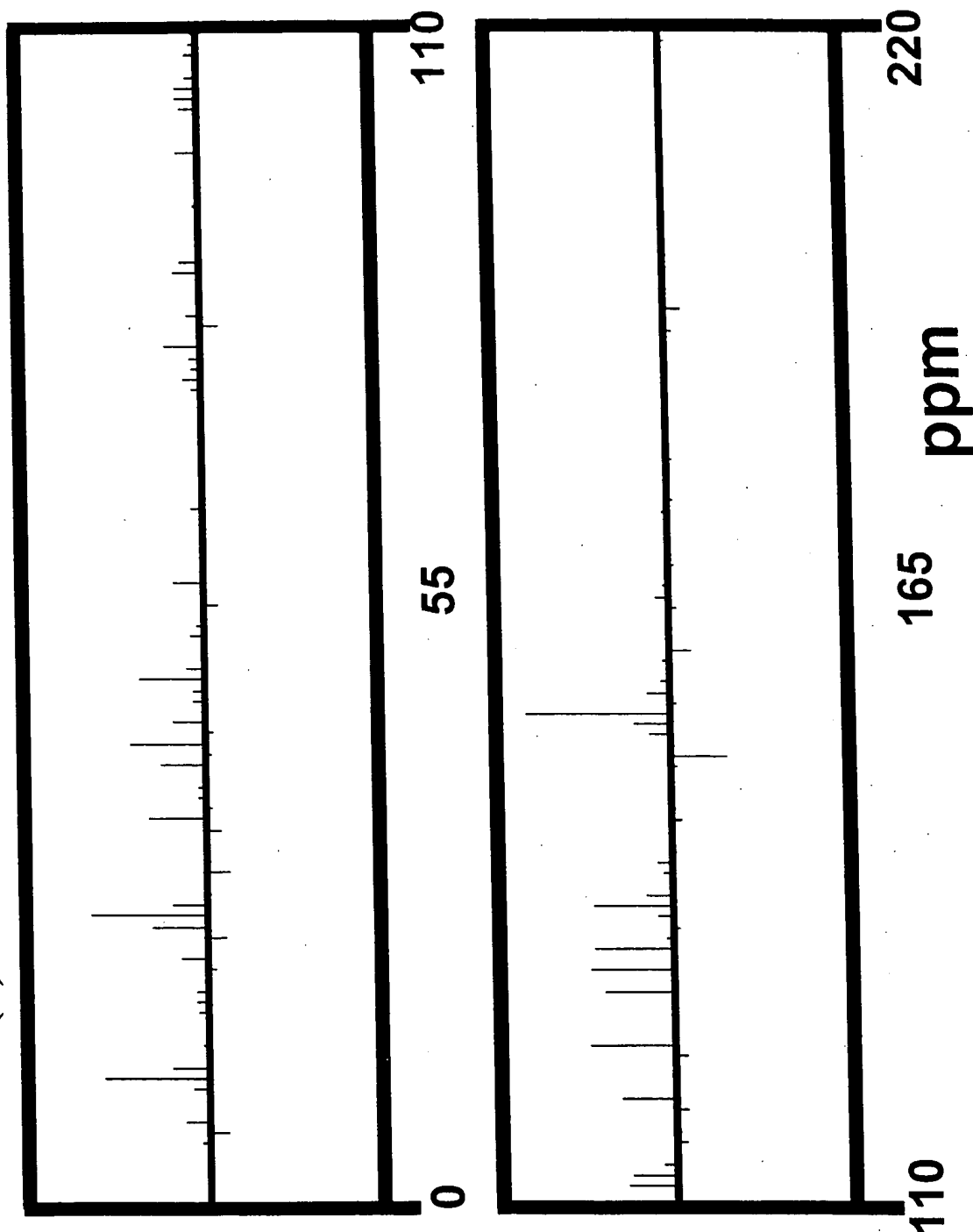


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Replacement Sheet (Sheet 15 of 31)

FIG. 12(a)



Relative Intensity



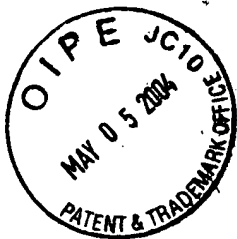
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Replacement Sheet (Sheet 16 of 31)

FIG. 12(b)





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Replacement Sheet (Sheet 17 of 31)

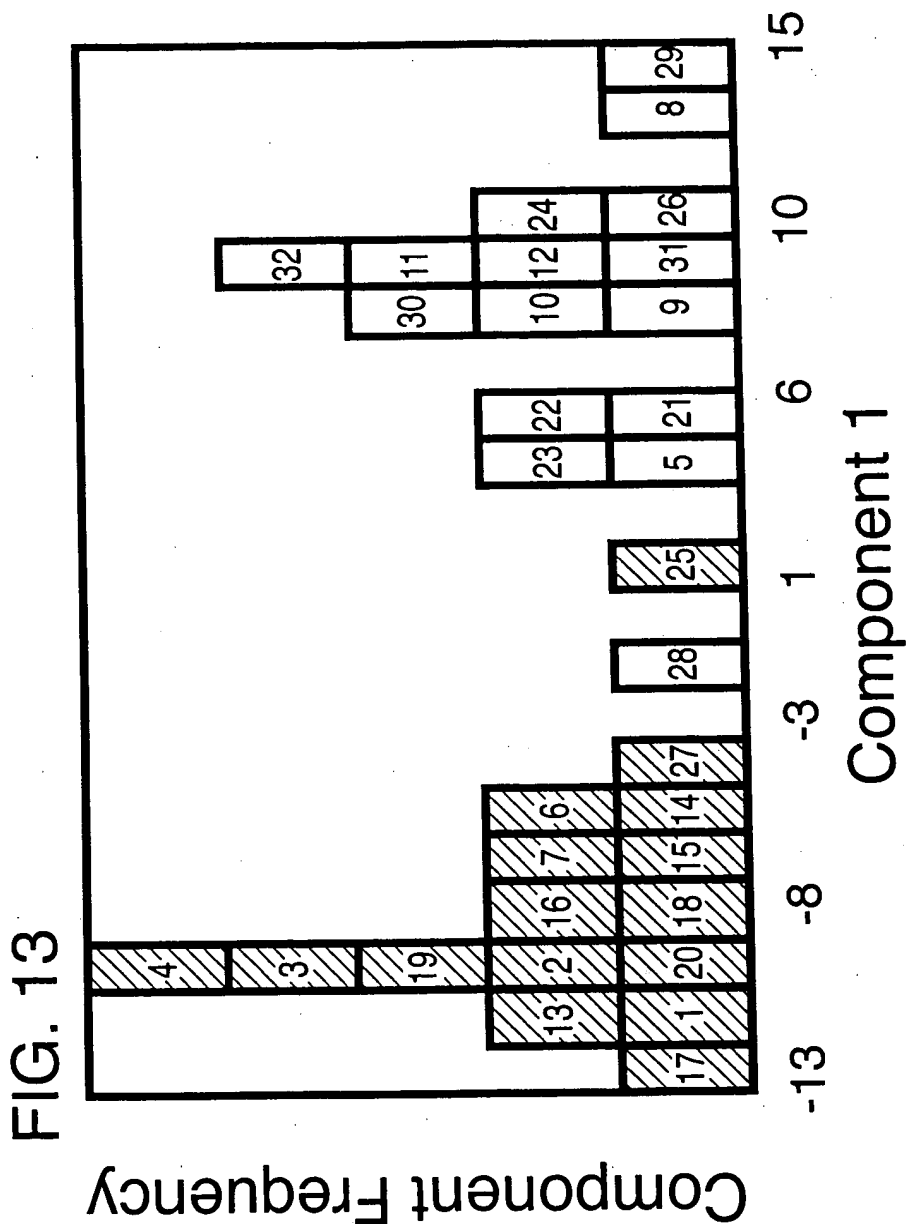
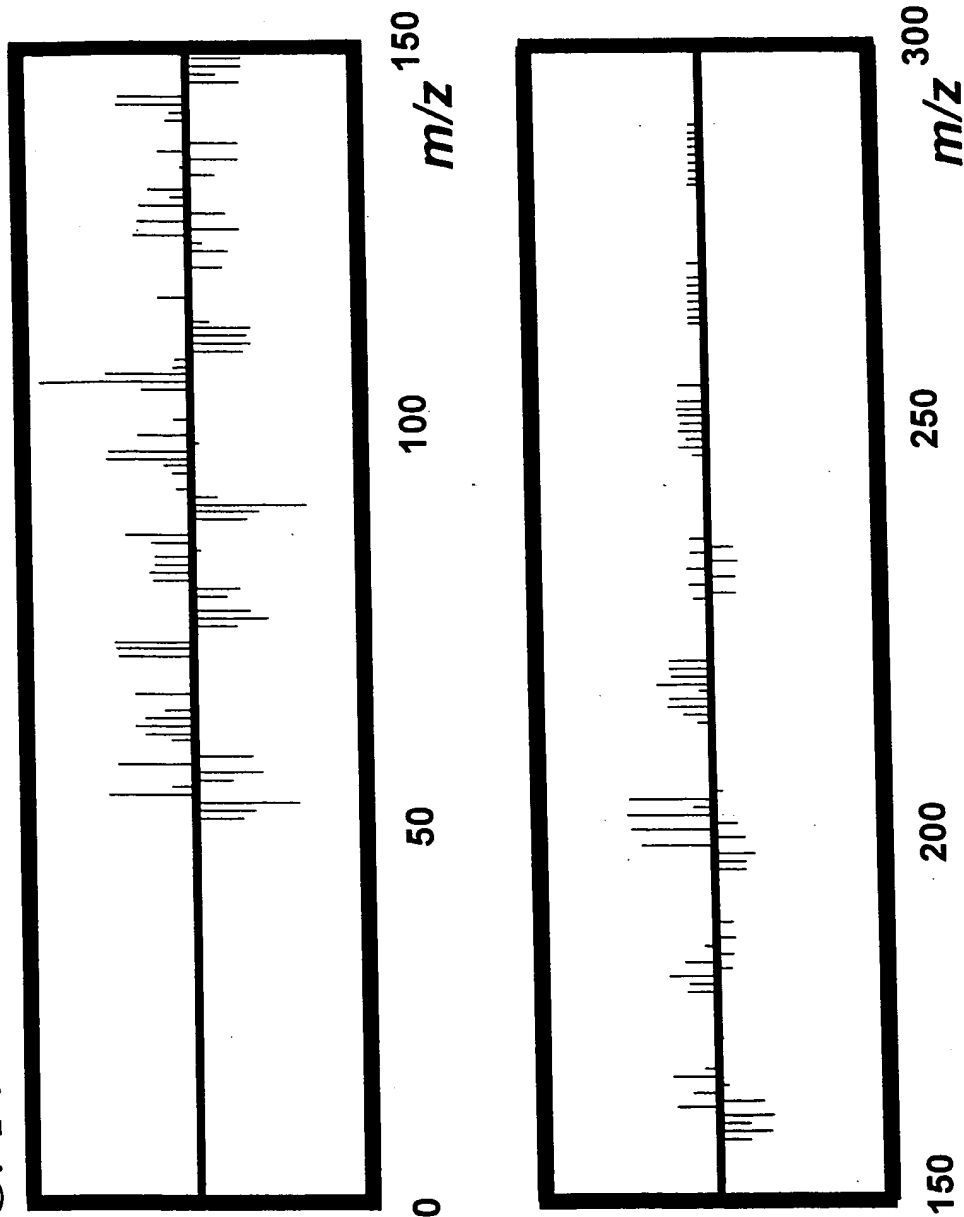
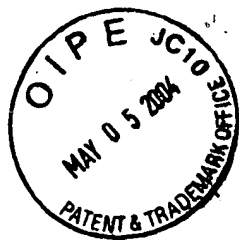


FIG. 14



Relative Intensity

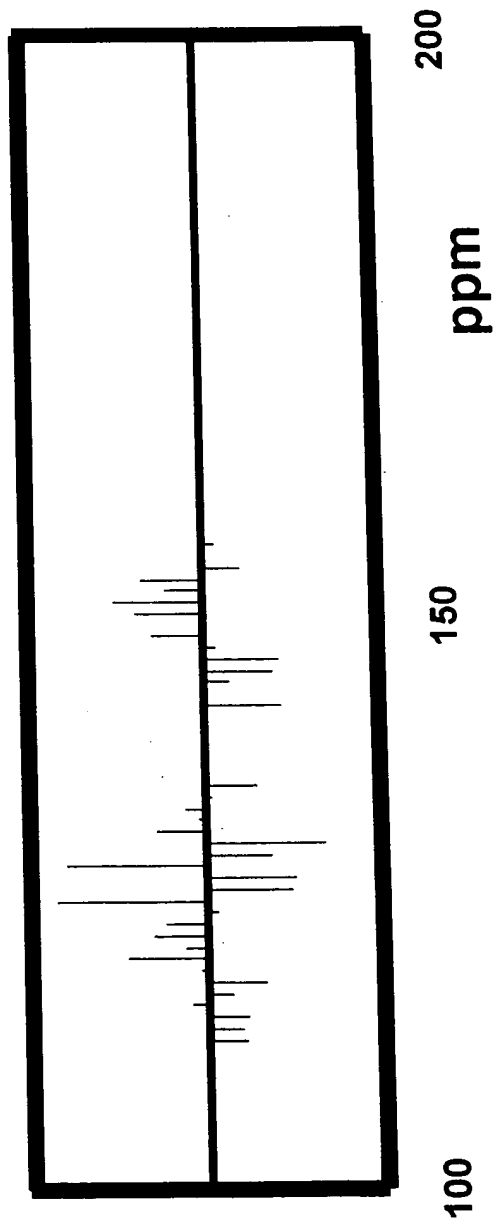


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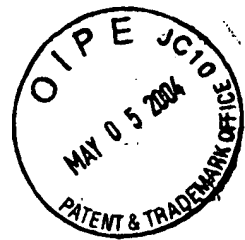
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Replacement Sheet (Sheet 19 of 31)

FIG. 15



Relative Intensity

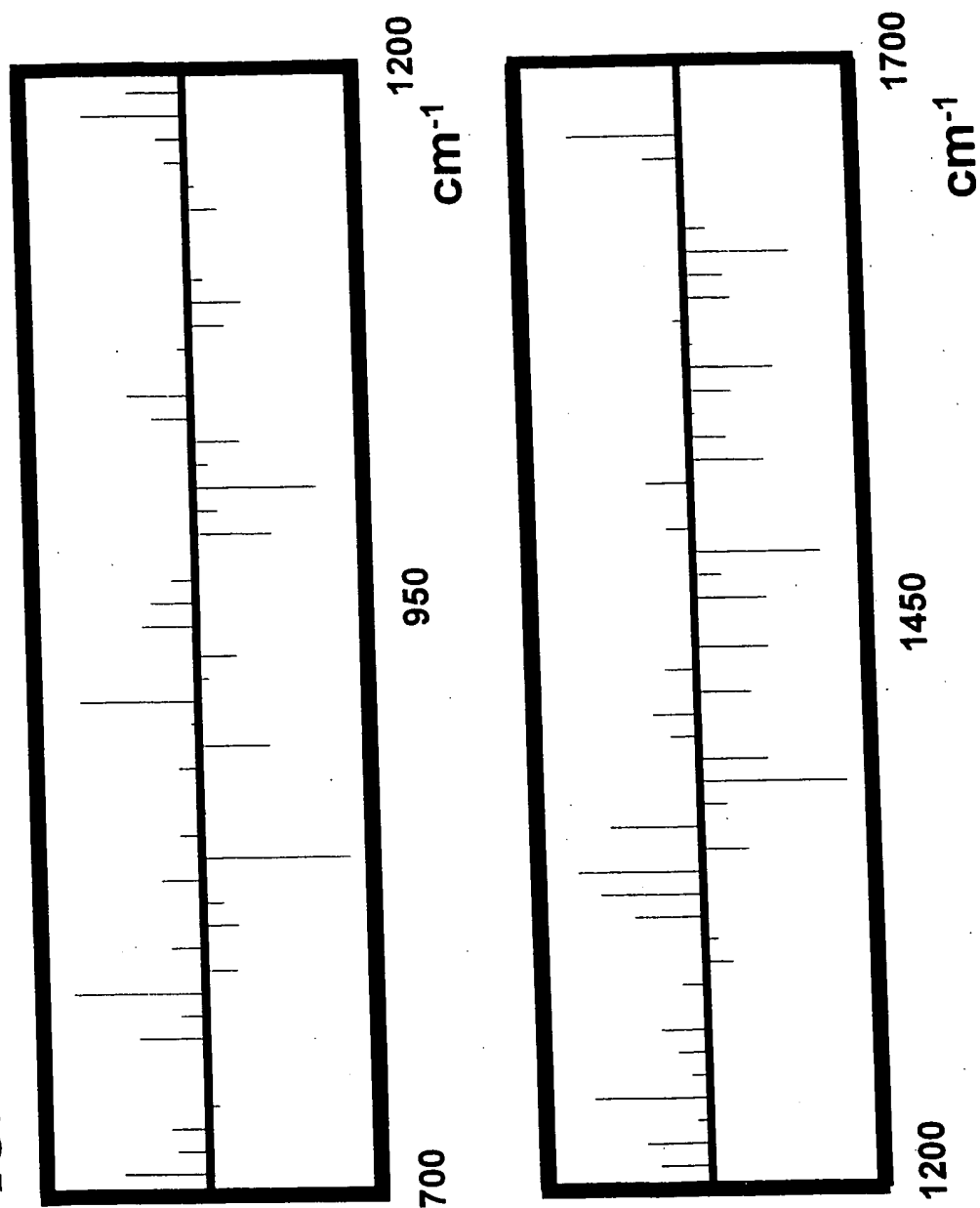


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Replacement Sheet (Sheet 20 of 31)

FIG. 16



Relative Intensity

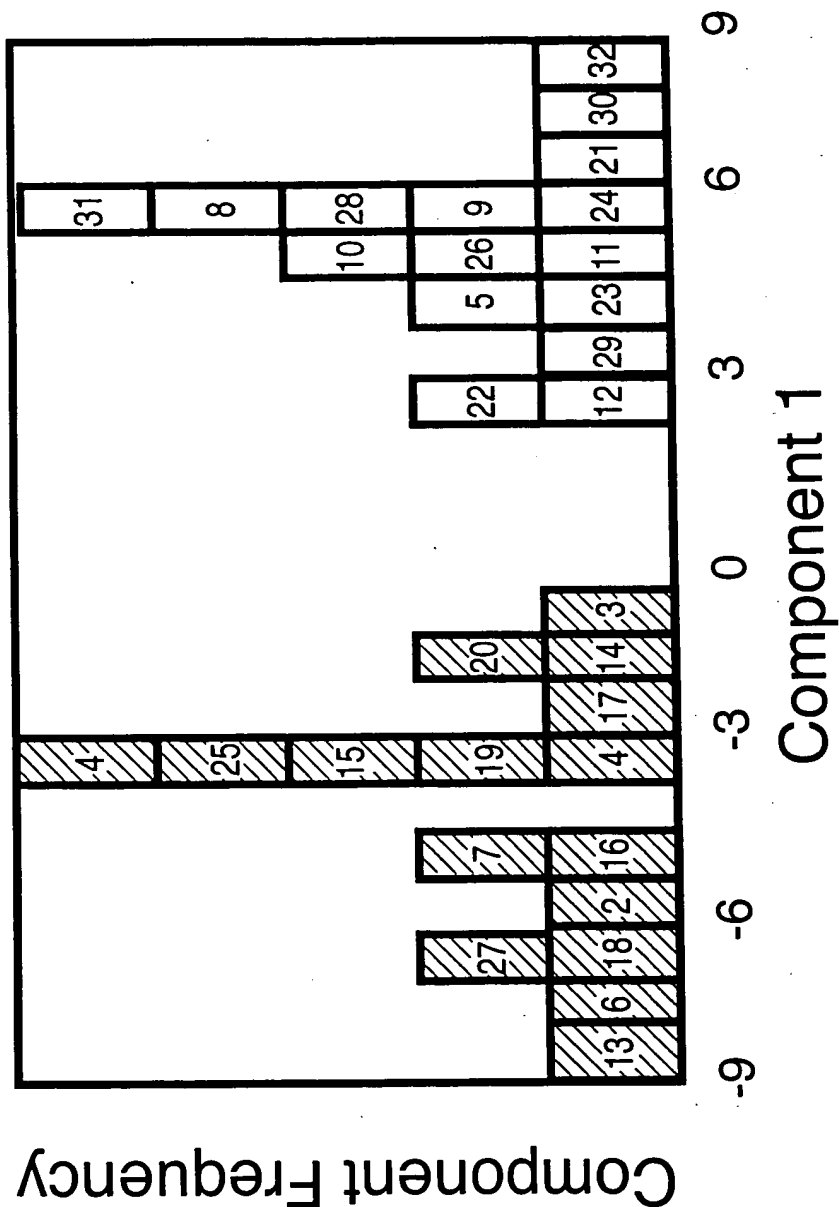


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Replacement Sheet (Sheet 21 of 31)

FIG. 17



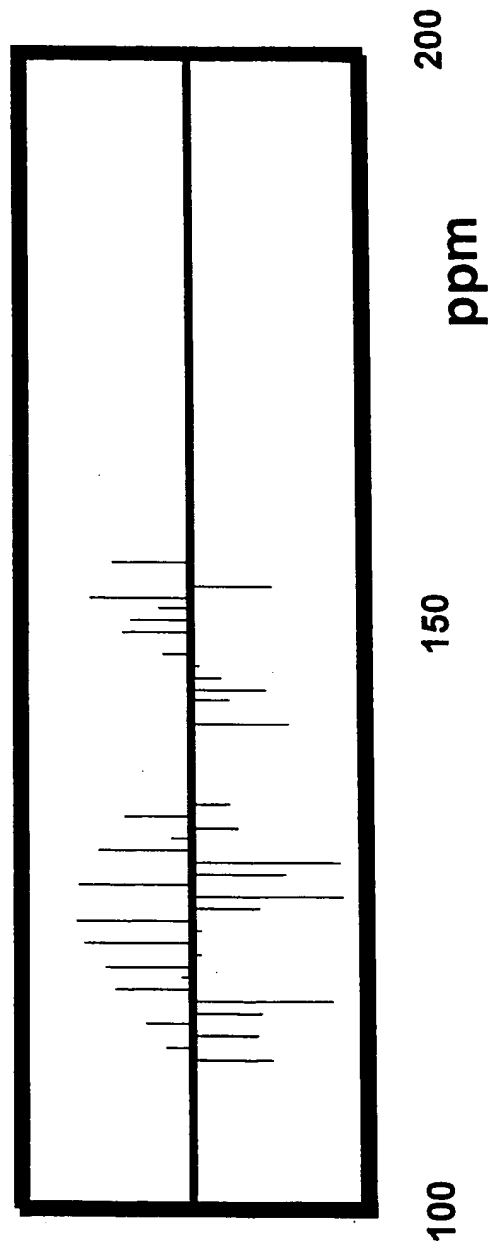


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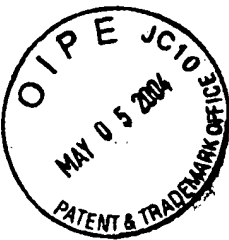
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Replacement Sheet (Sheet 22 of 31)

FIG. 18



Relative Intensity



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Replacement Sheet (Sheet 23 of 31)

FIG. 19

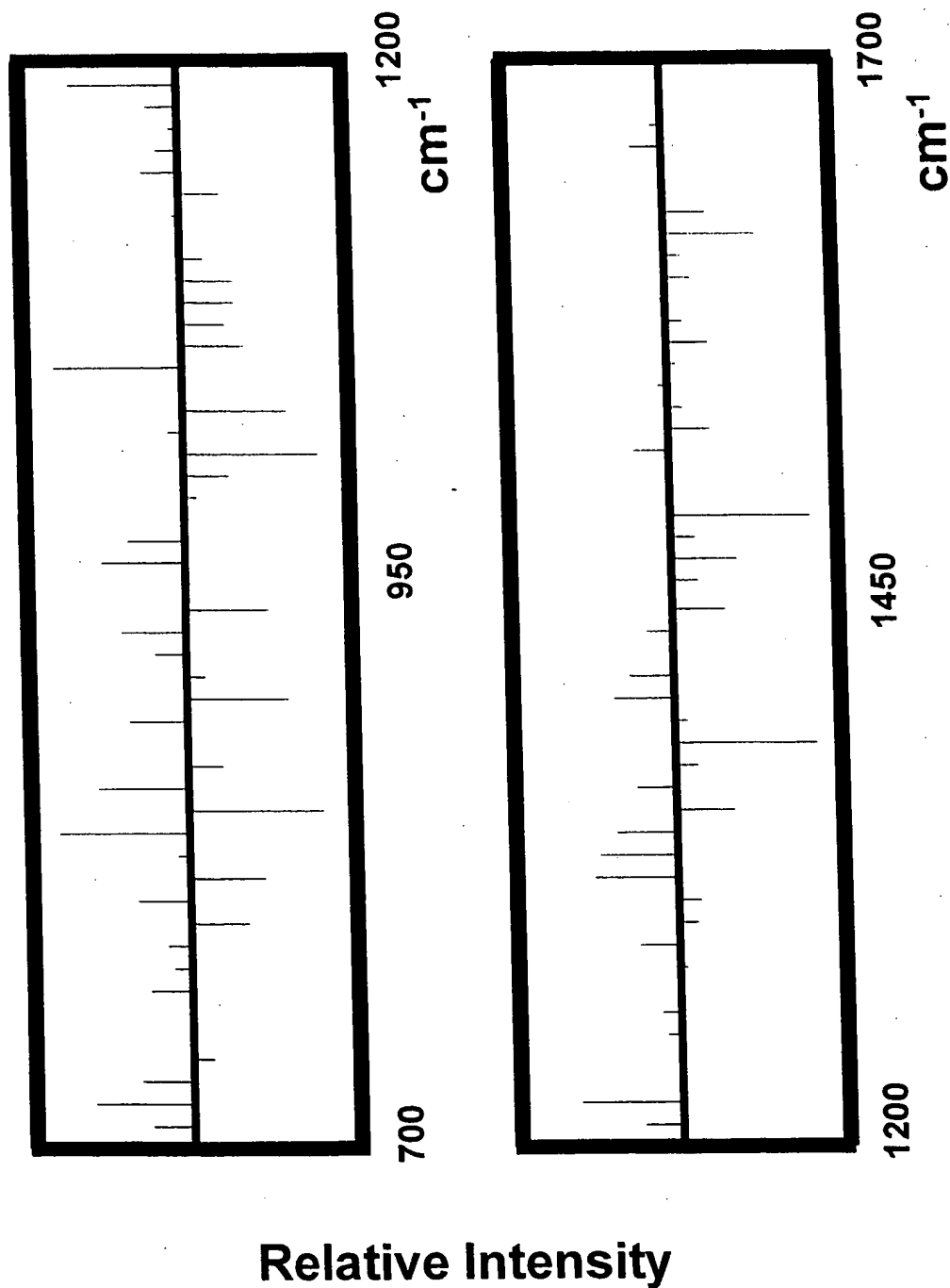
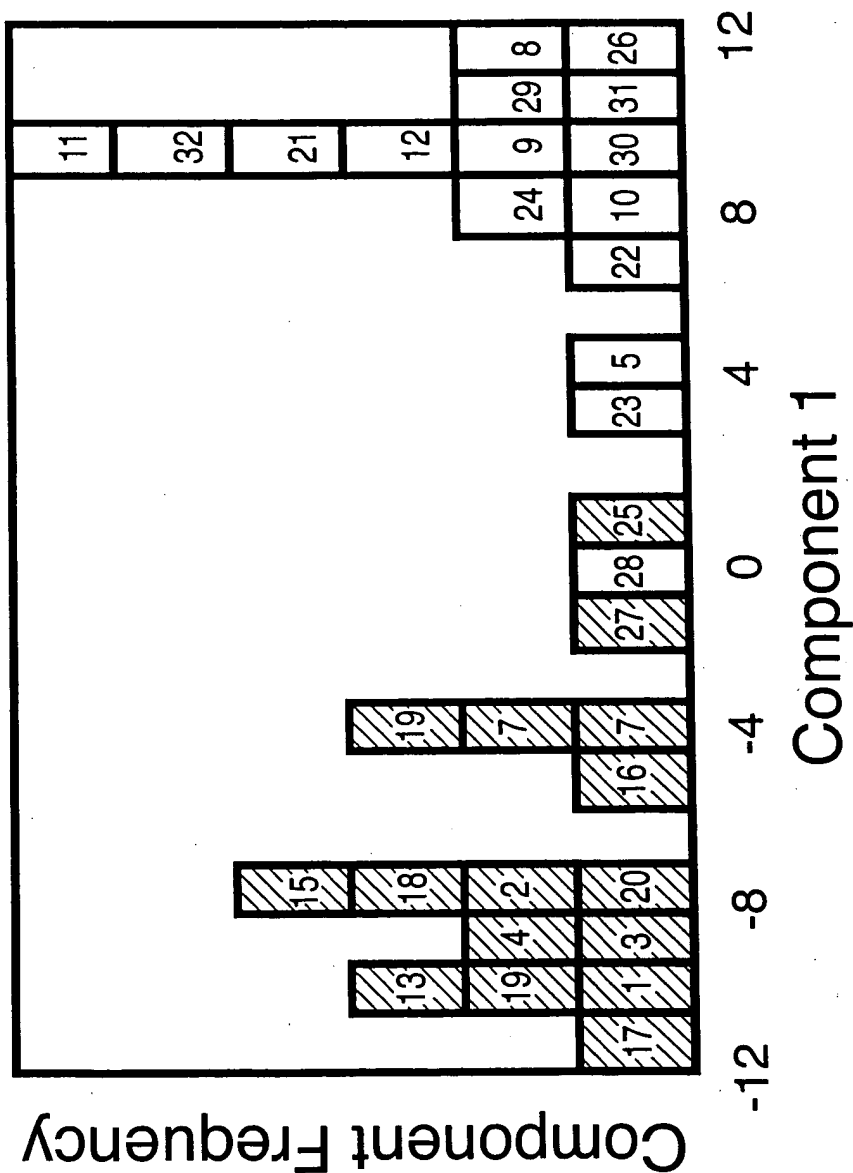
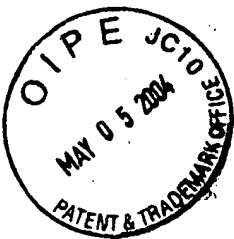


FIG. 20



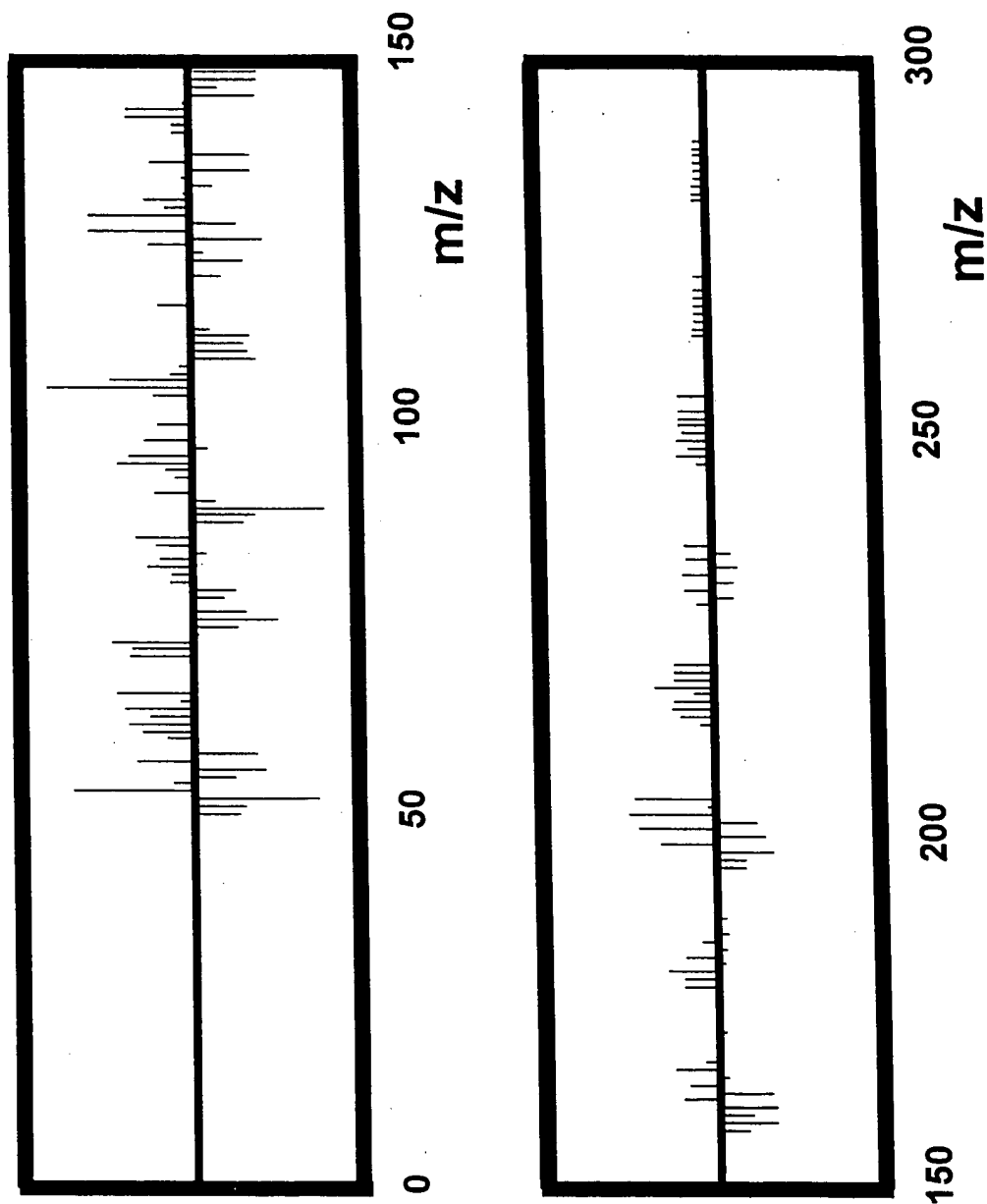


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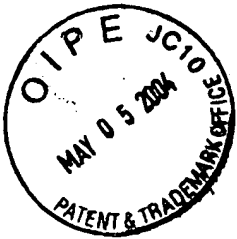
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Replacement Sheet (Sheet 25 of 31)

FIG. 21



Relative Intensity

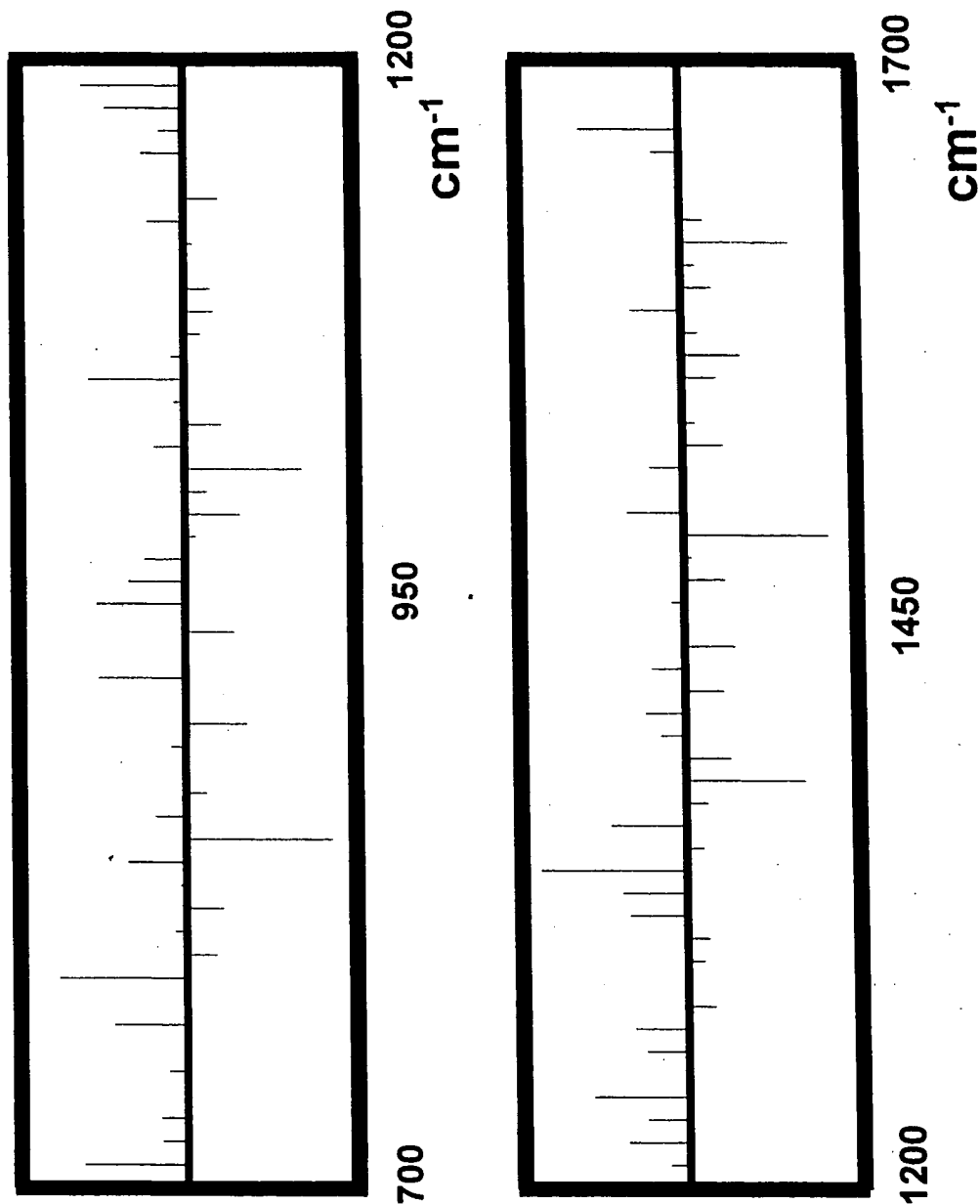


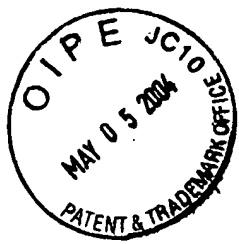
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Replacement Sheet (Sheet 26 of 31)

FIG. 22



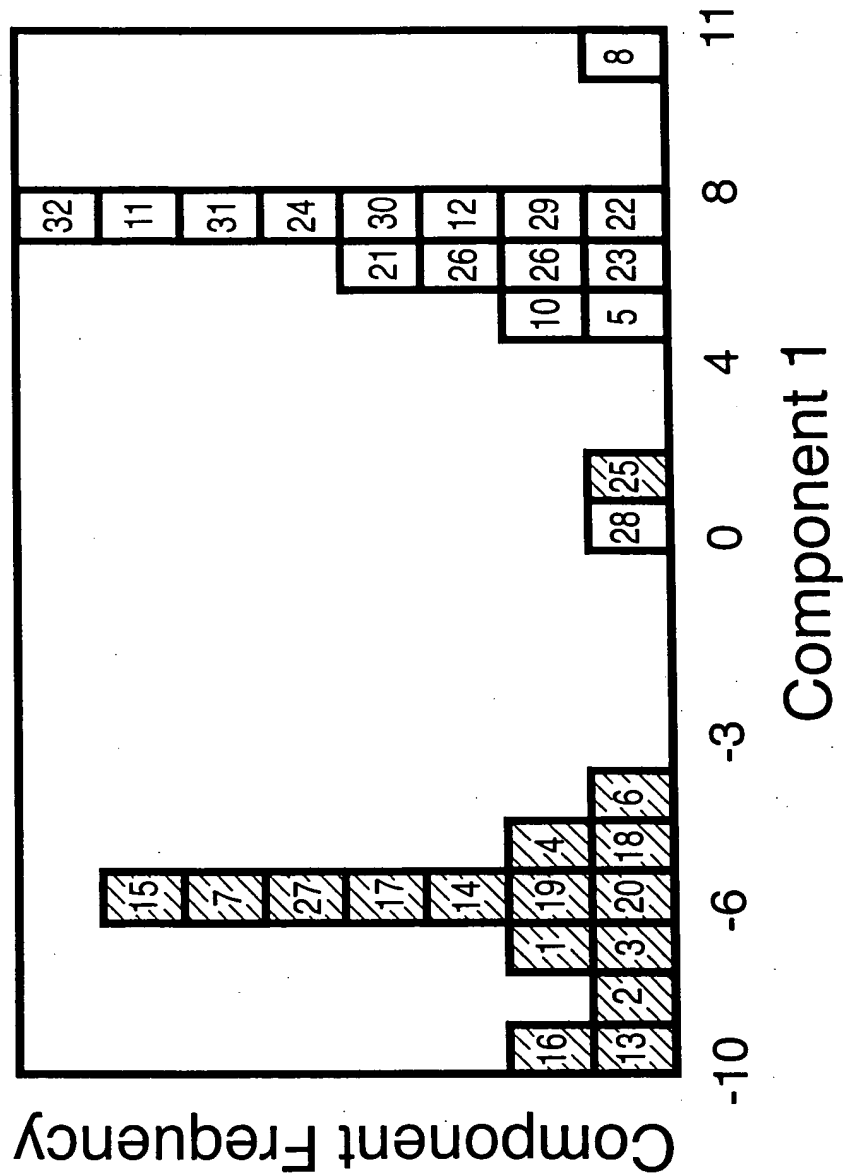


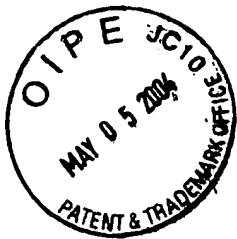
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 Filed: July 31, 2000

Replacement Sheet (Sheet 27 of 31)

FIG. 23



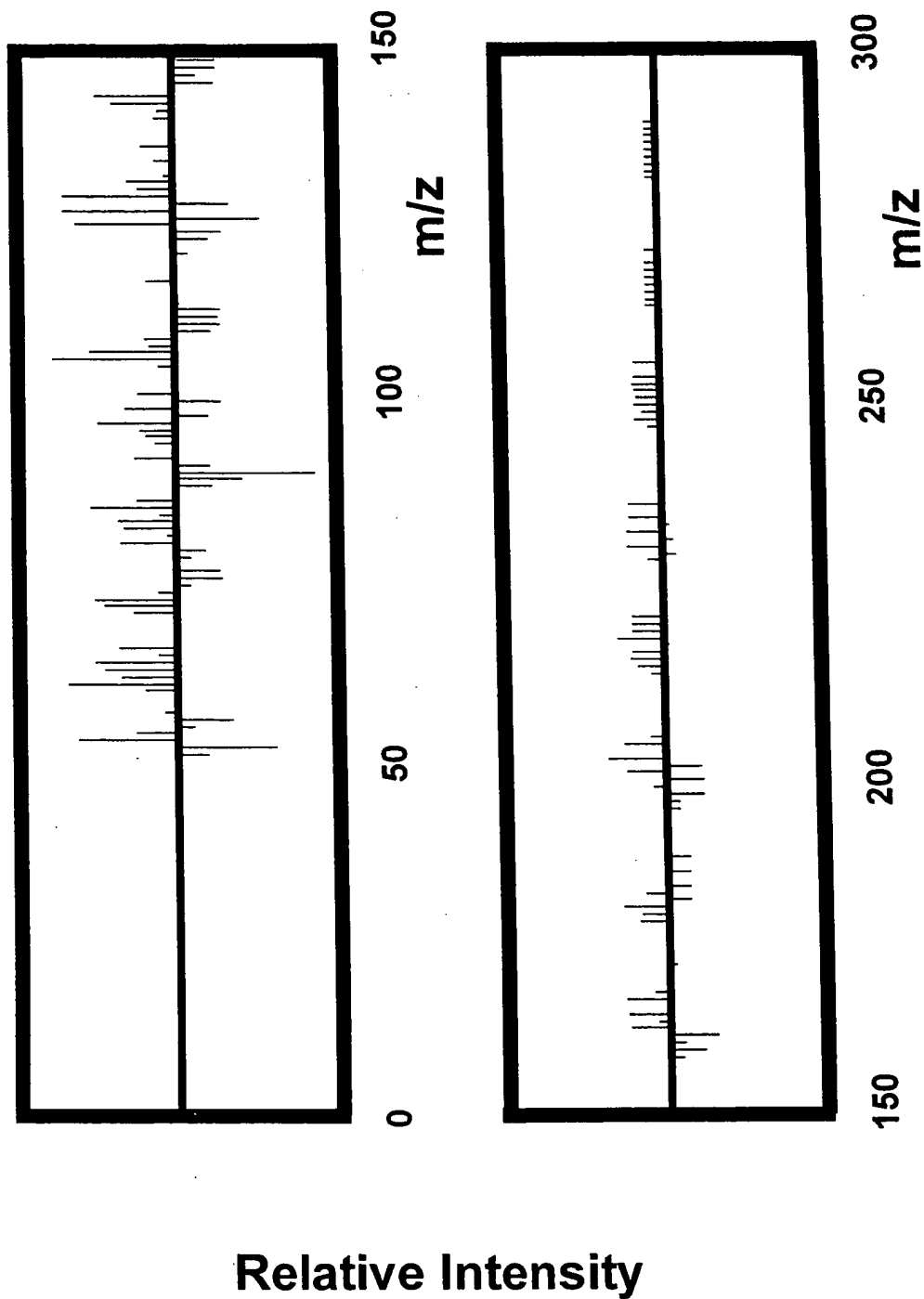


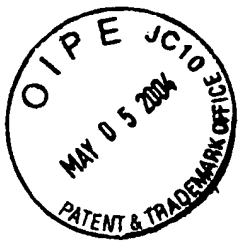
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Replacement Sheet (Sheet 28 of 31)

FIG. 24



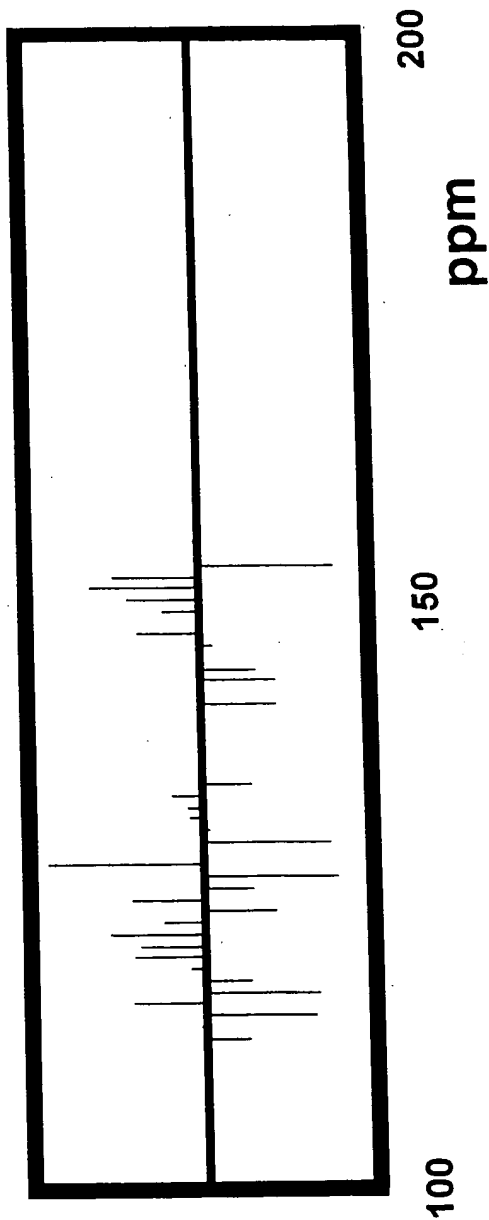


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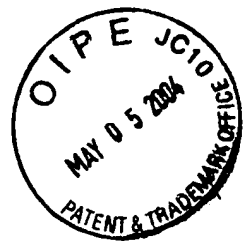
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Confirmation No. 4093
Filed: July 31, 2000

Replacement Sheet (Sheet 29 of 31)

FIG. 25



Relative Intensity



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Replacement Sheet (Sheet 30 of 31)

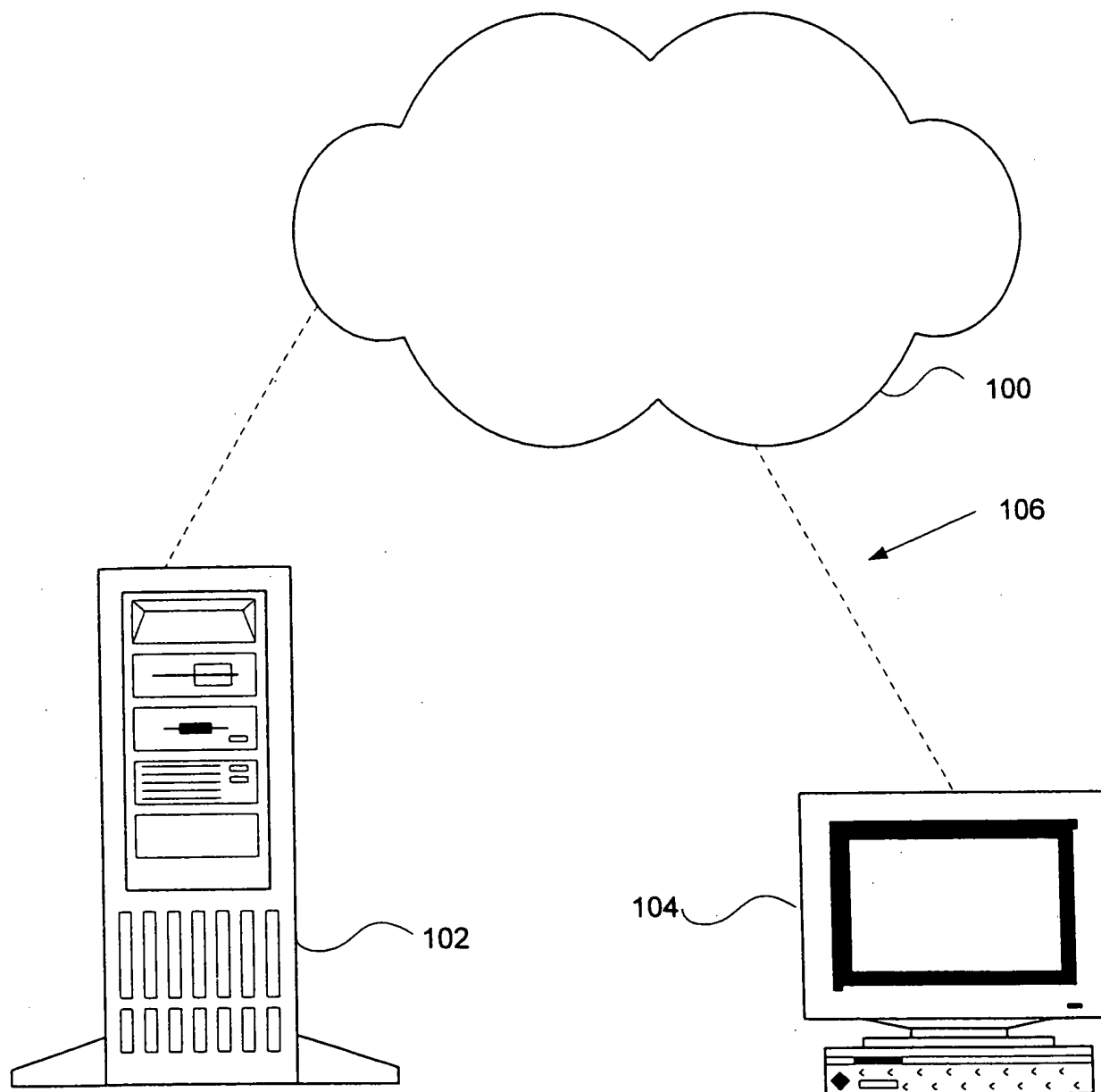
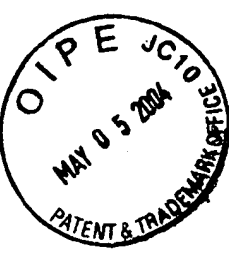


FIG. 26



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Replacement Sheet (Sheet 31 of 31)

FIG. 27

